Stacking Disorder in Hard Sphere Crystal under Gravity

Inst. of Technology and Science, Univ. Tokushima　Atsushi Mori,[1] Yoshihisa Suzuki

重力下の剛体球系結晶について、モンテカルロシミュレーションを行っている。まず、二層からなる双晶帯構造のスナップショットを示す。ショックレーの部分転位で端が終端された空孔原子型の積層欠陥と双晶構造について、弾性論の計算結果を示す。前者はグリシルであり、後者はセシルであることを示す結果が得られた。

1 Introduction

In 1997 Zhu *et al.* [1] opened a question that why the stacking disorder in the hard sphere (HS) colloidal crystal is reduced due to gravity. Though some experiments [2-5] have been performed thereafter, we have not yet reached the final conclusion.

Beside the above experiments, we have performed Monte Carlo simulations [6-8] using HS model. In this paper we concentrate on two stacking disorder structures. One is an intrinsic stacking fault with the Shockley partial dislocation terminating one of the ends. The other is a twin band structure. Elasticity calculations for those two structures are shown after showing snapshots of Monte Carlo simulations.

2 Monte Carlo Simulation

We have observed two types of stacking disorder. One is glissile, which is the intrinsic stacking structure. The other is sessile. There were, in appearance, and there can be, in principle, many structures possessing the sessile nature. Figure 1 is one of those; this picture result from overlay of two twin bands composed of two layers. We note that we this minimal twin band structure have been found to develop upward during the crystal growth [7].

We have also observed an intrinsic stacking fault [8]; transformation of the defective crystal in defect-less crystal [6] is caused by shrinkage of the intrinsic stacking fault.

3 Elasticity Calculation

In this paper we calculate the elastic strain energy separately from the gravitational energy. The strain energy due to a strait dislocation of Burgurs vector $\boldsymbol{b}$, which makes angle θ with respect to the dislocation

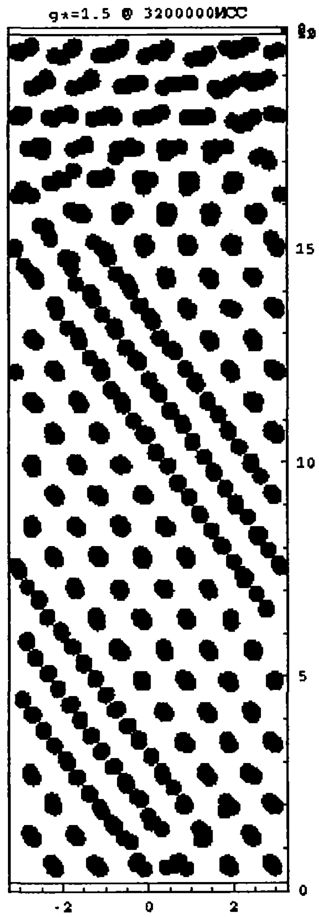

Figure 1: Projected snapshot of a sessile stacking disorder.

[1] E-mail: mori@opt.tokushima-u.ac.jp

line, is $W(R)=(\mu b^2/4\pi)[\cos^2\theta+\sin^2\theta/(1-\nu)]\ln(\alpha R/b)$ [9]. Here, R is the linear dimension over which the strain field expands, $\mu(\sim 10^2 k_B T/\sigma^3$ [10,11]) the shear modulus, ν the Poisson ratio, and α defines the dislocation core radius $r_0 = b/\alpha$. The elastic strain energy per unit length of the dislocation can be calculated by substituting $\boldsymbol{b}$ with $\boldsymbol{b}^1=(1/6)[\bar{2}11]$ and $\theta=\pi/6$. Addition of the core energy, stacking fault (interfacial) energy, and gravitational energy lead to the total energy, $U^{intr}=\left[(3/64\pi)\ln\left(\sqrt{6}\alpha R/a\right)+\beta/6\right]\mu a^2+\left(\varsigma\gamma_{sf}+mg/3\sigma\right)R$. Here, we have substituted 1/3 for ν for simplicity, and the core energy have been written as $\beta|\boldsymbol{b}^1|^2$ and the stacking fault energy $\varsigma\gamma_{sf}R$ with β and ς being constants ($\gamma_{st}\sim 10^{-4}k_B T/\sigma^4$ [12]), the gravitational contribution $mgR/3\sigma$, a is the face-centered cubic (fcc) lattice constant, and σ, the HS diameter, defines the unit length.

For minimal twin band structure, the partial dislocation on the one of two lattice planes in the twin band can be regarded to have opposite Burgers vector to the other due to the periodicity of fcc. That is, a dislocation dipole forms at the end of this (minimal or two plane thick) twin band structure. It means the cancellation of the long-range (logarithmic) strain energy. The total energy may be written as $U^{twin}=9\beta'/2\,\mu a^2+\left(3\varsigma'\gamma_{sf}+mg/\sigma\right)R$ in the same manner as for the intrinsic stacking fault.

4 Concluding Remark

Vanishing logarithmic term suggests the sessile nature, i.e., the end of the minimal twin band structure hardly glides, in contrast to the intrinsic stacking fault [8]. We anticipate that premelting near a defect [10] may mediate the shrinkage of the sessile structure.

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